Band structure of bismuth, antimony and some other elemental crystals

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This collection of band structures intends to supplement the *Handbook of the Band Structure of Elemental Solids* by Dimitris A. Papaconstantopoulos wherever the band structures of that book do not assume the commonly occuring allotrope of the given element.

A physicist looking for a quick and reliable reference on band structure of elemental substances may naturally go fetch the book mentioned in the abstract:[1] just as we did recently when dealing with certain aspects of transport in bismuth. It turns out, however, that some elements have band structures calculated in that book only for unrealistic (or at least not very common) crystal structure. To that end, the mentioned example (bismuth, see p. 373) is calculated for simple cubic structure (see also intro to Ch. 9 on p. 359) and that is not very helpful in contemplating devices containing thin layers of bismuth grown under ordinary conditions.[2]

While for bismuth, it was a matter of a quick literature search to find calculated band structure of the naturally most abundant allotrope (space group $R\bar{3}m$) we soon came across another element, antimony where the search for published results proved to be more tedious. Assuming that other researchers may find themselves in a similar situation, we decided to submit this short article to `arxiv.org` for the sake of convenience of others and our own. We intend to expand this collection as time goes by other elemental solids and welcome suggestions from the broad audience of the preprint server for including further elemental systems.

On technical side, we use density functional theory (DFT) in linear augmented plane wave (LAPW) method as implemented in `Wien2k` package.[3] Some brief comments about the calculation itself are given, as we deemed necessary, in each subsequent section but we do not aspire by any means to perform an exhaustive and/or highly accurate study of band structures. The sole intention was to prepare a quick and accessible reference for the basic character of the band structure in the selected elemental solids.

I. BISMUTH

A prototypical semimetal, where hole pockets are located around T and and electron pockets around L, see Fig. 1. Here, GGA was used and the effect of spin orbit interaction is important, as it helps opening gaps close to the Fermi level. More careful calculations (including GW) and Brillouin zone (BZ) plot can be found in Aguilera et al. [4] (note that in Fig. 2 of that reference, two W points were considered which are not identical and Fig. 1 therefore adds another leg to the path through the BZ). Lattice constants and atomic positions[5] are given in Tab. I, the rhombohedral $A7$ structure is commented on in Sec. III.

II. ANTIMONY

Semimetallic band structure with electron pockets at the L point of the rhombohedric Brillouin zone (RHL_1 according to Ref. 6) is shown in Fig. 2 for GGA and lattice parameters of Ref. [7] (see Sec. III for a summary). Apart from a qualitative description of the band structure[8] we have not found any up-to-date *ab initio* calculation and suggestions for good references will be appreciated.

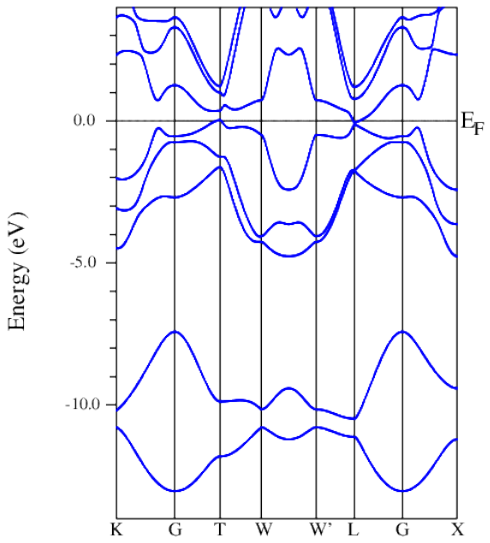

FIG. 1. Bismuth.

III. CRYSTAL STRUCTURE DETAILS

General remarks plus tables of structural parameters used for calculations in this article are collected here. Lattice constants and atomic positions for Bi, Sb, and Te crystals are given in Table I.

In order to follow the convention of `Wien2k` (Ref. 3) input files, rhombohedral lattices must have the hexagonal unit cell parameters specified in the input file, while the atomic positions used must be given in the rhombohedral representation. Hence, both the hexagonal and rhombohedral configurations are given in Table I for Bi and Sb.

Fig. 3 shows the relation between the hexagonal and the rhombohedral configurations. Bi and Sb crystal structures have the same symmetry, the difference being the values of the unit cell parameters and the z component of the atomic positions (compare Table I and Fig. 3).

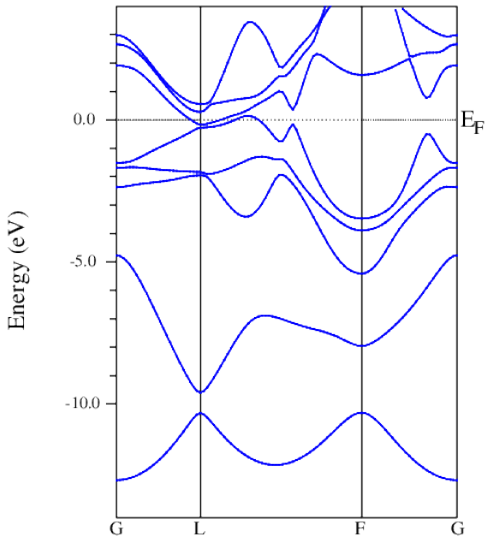

FIG. 2. Antimony.

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[1] Dimitris A. Papaconstantopoulos: *Handbook of the Band Structure of Elemental Solids* (Springer, 2nd Edition) 2015.
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TABLE I. Crystal structure of bismuth,[5] antimony,[7] and tellurium.[9]

Bi - hexagonal configuration		**rhombohedral configuration**
a, c (Å)	4.546(2), 11.862(6)	4.7458(19)
V (Å^3)	212.30(17)	70.77(7)
Space group	$R\bar{3}m$	
	atomic positions	
Bi1	(0,0,0.23389(2))	(0.234,0.234,0.234)
Bi2		(0.766,0.766,0.766)
Sb - hexagonal configuration		**rhombohedral configuration**
a, c (Å)	4.30724, 11.2754(6)	4.5067
V (Å^3)	181.16(1)	
Space group	$R\bar{3}m$	
	atomic positions	
Sb1	(0,0,0.2664(1))	(0.2664,0.2664,0.2664)
Sb2		(0.7336,0.7336,0.7336)
Te		
a, c (Å)	4.4593(2), 5.9282(4)	
V (Å^3)	102.094(9)	
Space group	$P3121$	
	atomic position	
Te	(0.261969,0,0.3333)	

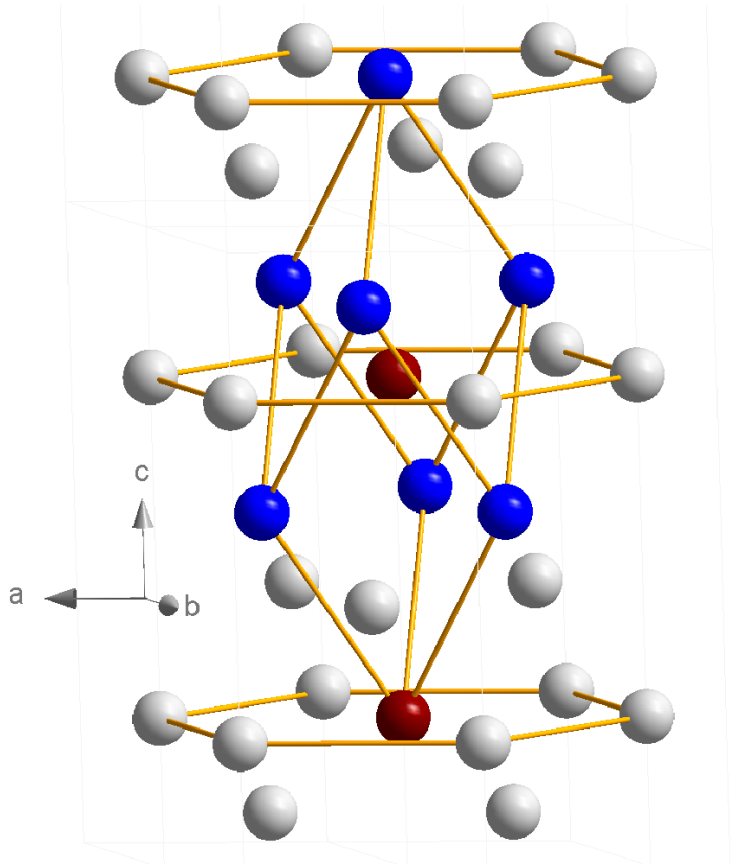

FIG. 3. Schematic relation between the hexagonal and rhombohedral configurations. Coloured atoms belong to the latter and the ones highlighted in red correspond to the positions (e.g. Bi1, Bi2) given in Tab. I.